



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2017 – 10:28 PM EST

PDB ID : 4PDC
Title : Crystal structure of Cowpox virus CPXV018 (OMCP) bound to human NKG2D
Authors : Lazear, E.; Nelson, C.A.; Fremont, D.H.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : unknown
Resolution : 1.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

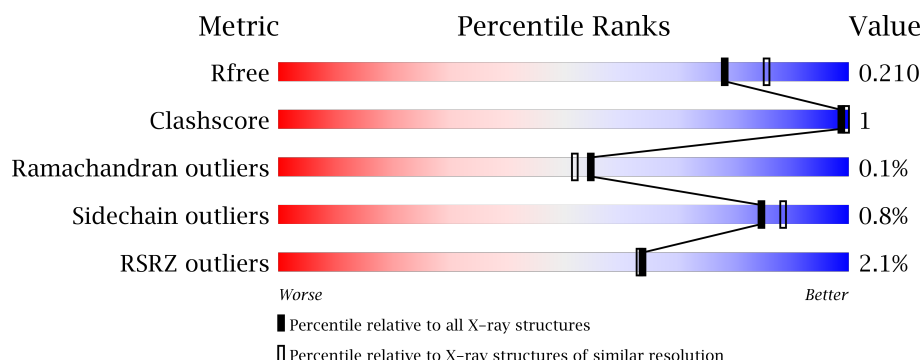
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	123	<div> <div>5%</div> <div>95%</div> <div>5%</div> </div>
1	B	123	<div> <div>3%</div> <div>97%</div> <div>..</div> </div>
1	C	123	<div> <div>98%</div> <div>.</div> </div>
1	D	123	<div> <div>5%</div> <div>95%</div> <div>5%</div> </div>
2	E	150	<div> <div>99%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	150	<div><div></div><div>%</div><div>99%</div><div>.</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13255 atoms, of which 6104 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NKG2-D type II integral membrane protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	123	Total	C	H	N	O	S	0	0	0
			1931	633	935	160	191	12			
1	B	122	Total	C	H	N	O	S	0	0	0
			1916	628	929	159	188	12			
1	C	123	Total	C	H	N	O	S	0	0	0
			1931	633	935	160	191	12			
1	D	123	Total	C	H	N	O	S	0	0	0
			1931	633	935	160	191	12			

- Molecule 2 is a protein called CPXV018 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	150	Total	C	H	N	O	S	0	0	0
			2443	805	1185	200	247	6			
2	F	150	Total	C	H	N	O	S	0	0	0
			2443	805	1185	200	247	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP Q8QN43
E	23	ASP	TYR	engineered mutation	UNP Q8QN43
E	95	ASP	PHE	engineered mutation	UNP Q8QN43
F	0	GLY	-	expression tag	UNP Q8QN43
F	23	ASP	TYR	engineered mutation	UNP Q8QN43
F	95	ASP	PHE	engineered mutation	UNP Q8QN43

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		

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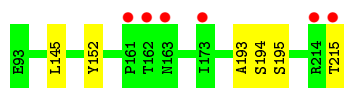
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	85	Total 85	O 85	0	0
3	C	87	Total 87	O 87	0	0
3	D	96	Total 96	O 96	0	0
3	E	165	Total 165	O 165	0	0
3	F	137	Total 137	O 137	0	0

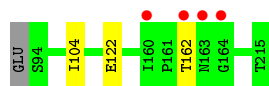
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NKG2-D type II integral membrane protein



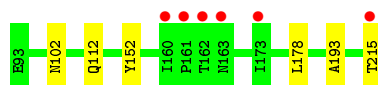
- Molecule 1: NKG2-D type II integral membrane protein



- Molecule 1: NKG2-D type II integral membrane protein



- Molecule 1: NKG2-D type II integral membrane protein

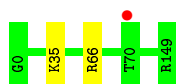


- Molecule 2: CPXV018 protein



- Molecule 2: CPXV018 protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.31Å 101.11Å 91.37Å 90.00° 91.63° 90.00°	Depositor
Resolution (Å)	45.66 – 1.99 45.67 – 1.99	Depositor EDS
% Data completeness (in resolution range)	92.9 (45.66-1.99) 90.4 (45.67-1.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.166 , 0.214 0.166 , 0.210	Depositor DCC
R_{free} test set	1938 reflections (3.98%)	DCC
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.128 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13255	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/1024	0.41	0/1388
1	B	0.25	0/1015	0.44	0/1376
1	C	0.25	0/1024	0.41	0/1388
1	D	0.25	0/1024	0.41	0/1388
2	E	0.26	0/1291	0.44	0/1745
2	F	0.26	0/1291	0.42	0/1745
All	All	0.25	0/6669	0.42	0/9030

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	996	935	933	3	0
1	B	987	929	927	1	0
1	C	996	935	933	2	0
1	D	996	935	933	2	0
2	E	1258	1185	1182	1	0
2	F	1258	1185	1182	1	0
3	A	90	0	0	0	0
3	B	85	0	0	0	0
3	C	87	0	0	1	2
3	D	96	0	0	0	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	165	0	0	0	0
3	F	137	0	0	0	0
All	All	7151	6104	6090	8	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (8) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ASN:O	1:D:112:GLN:NE2	2.46	0.49
1:C:185:GLN:HG2	2:F:66:ARG:NH2	2.30	0.47
1:C:185:GLN:OE1	3:C:362:HOH:O	2.21	0.45
1:A:152:TYR:CD2	1:A:193:ALA:HB2	2.52	0.45
1:A:145:LEU:HD13	1:B:104:ILE:HD11	2.00	0.42
1:D:152:TYR:CD2	1:D:193:ALA:HB2	2.54	0.42
2:E:78:THR:HB	2:E:97:LEU:HB2	2.02	0.41
1:A:194:SER:HA	1:A:195:SER:HA	1.86	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:301:HOH:O	3:D:306:HOH:O[1_655]	2.15	0.05
3:C:318:HOH:O	3:D:306:HOH:O[1_655]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	121/123 (98%)	117 (97%)	4 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	120/123 (98%)	115 (96%)	4 (3%)	1 (1%)	22	15
1	C	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
1	D	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
2	E	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
2	F	148/150 (99%)	144 (97%)	4 (3%)	0	100	100
All	All	779/792 (98%)	758 (97%)	20 (3%)	1 (0%)	55	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	162	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/113 (100%)	112 (99%)	1 (1%)	82	87
1	B	112/113 (99%)	111 (99%)	1 (1%)	82	87
1	C	113/113 (100%)	112 (99%)	1 (1%)	82	87
1	D	113/113 (100%)	111 (98%)	2 (2%)	64	68
2	E	142/142 (100%)	142 (100%)	0	100	100
2	F	142/142 (100%)	141 (99%)	1 (1%)	87	90
All	All	735/736 (100%)	729 (99%)	6 (1%)	85	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	THR
1	B	122	GLU
1	C	145	LEU
1	D	178	LEU
1	D	215	THR

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Mol	Chain	Res	Type
2	F	35	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	109	ASN
1	D	177	ASN
2	F	88	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	123/123 (100%)	-0.04	6 (4%) 30 30	14, 25, 62, 102	0
1	B	122/123 (99%)	-0.07	4 (3%) 47 47	14, 25, 57, 93	0
1	C	123/123 (100%)	-0.17	0 100 100	13, 23, 41, 61	0
1	D	123/123 (100%)	0.06	6 (4%) 30 30	14, 26, 60, 115	0
2	E	150/150 (100%)	-0.27	0 100 100	13, 21, 40, 68	0
2	F	150/150 (100%)	-0.20	1 (0%) 87 87	13, 22, 48, 66	0
All	All	791/792 (99%)	-0.12	17 (2%) 64 63	13, 23, 51, 115	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	161	PRO	4.2
1	A	173	ILE	3.9
1	B	162	THR	3.2
1	B	164	GLY	3.1
1	B	163	ASN	3.1
1	A	215	THR	2.9
1	D	162	THR	2.6
1	A	161	PRO	2.6
1	D	173	ILE	2.5
1	D	215	THR	2.3
1	D	163	ASN	2.3
1	A	214	ARG	2.3
2	F	70	THR	2.2
1	A	162	THR	2.2
1	B	160	ILE	2.2
1	D	160	ILE	2.2
1	A	163	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.